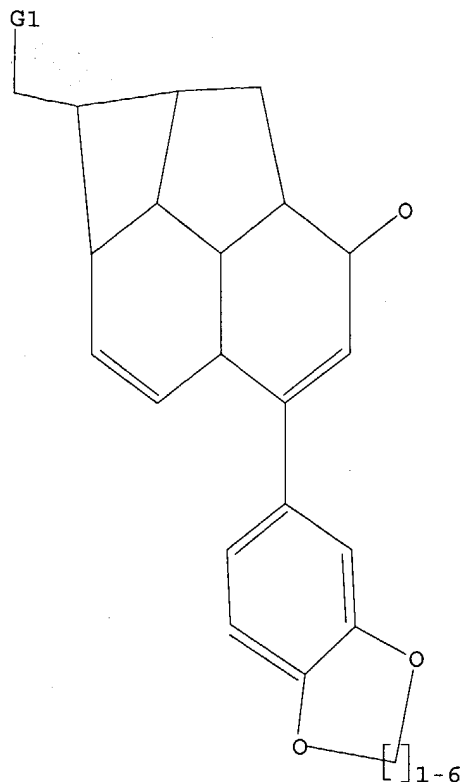


9/28/2004

STR



G1 PhO, COOH, CHO, C(O)CH₃, NH₂, NO₂, Cb, Hy, Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss full

FULL SEARCH INITIATED 14:52:58 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 1191 TO ITERATE

100.0% PROCESSED 1191 ITERATIONS

1 ANSWERS

SEARCH TIME: 00.00.01

L2 1 SEA SSS FUL L1

=> d l2 iall

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN

RN 660857-93-2 REGISTRY

ED Entered STN: 10 Mar 2004

CN 1H-Cyclobut[bc]acenaphthylene-1-acetic acid, 5-(1,3-benzodioxol-5-yl)-
1a,2,2a,3,5a,7a,7b,7c-octahydro-3-hydroxy-, (1S,1aR,2aR,3S,5aR,7aR,7bS,7cS)
)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN Endiandric acid H

FS STEREOSEARCH

MF C22 H22 O5

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

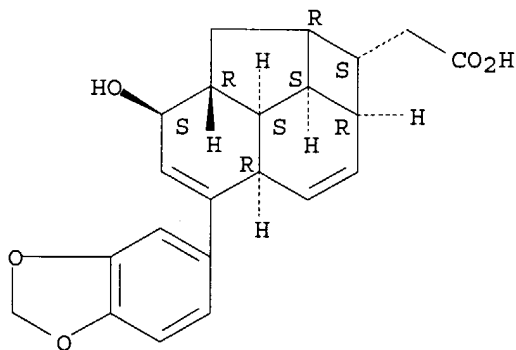
DT.CA CAplus document type: Patent

RL.P Roles from patents: BIOL (Biological study); OCCU (Occurrence); PREP
(Preparation); PRP (Properties); USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3O2-C6	OCOC2-C6	5-6	C7O2	333.584.8	1
C4-C5-C6-C6	C4-C5-C6-C6	4-5-6-6	C13	1825.2.6	1

Absolute stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	63.7	pH 1	(1) ACD
Bioconc. Factor (BCF)	50.6	pH 4	(1) ACD
Bioconc. Factor (BCF)	1	pH 7	(1) ACD
Bioconc. Factor (BCF)	1	pH 8	(1) ACD
Bioconc. Factor (BCF)	1	pH 10	(1) ACD
Boiling Point (BP)	576.2+/-50.0 deg C	760 Torr	(1) ACD
Enthalpy of Vap. (HVP)	90.77+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	206.9+/-42.5 deg C		(1) ACD
Freely Rotatable Bonds (FRB)	5		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	2		(1) ACD
Koc (KOC)	680	pH 1	(1) ACD
Koc (KOC)	540	pH 4	(1) ACD
Koc (KOC)	2.67	pH 7	(1) ACD
Koc (KOC)	1	pH 8	(1) ACD
Koc (KOC)	1	pH 10	(1) ACD
logD (LOGD)	2.68	pH 1	(1) ACD
logD (LOGD)	2.58	pH 4	(1) ACD
logD (LOGD)	0.27	pH 7	(1) ACD
logD (LOGD)	-0.66	pH 8	(1) ACD
logD (LOGD)	-1.40	pH 10	(1) ACD
logP (LOGP)	2.677+/-0.383		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	>=0.1 - <1 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	366.41		(1) ACD

pKa (PKA)	4.59+/-0.20	Most Acidic	(1) ACD
Vapor Pressure (VP)	4.07E-14 Torr	25 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software
Solaris V4.76 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

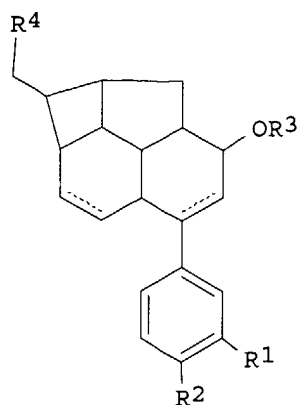
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

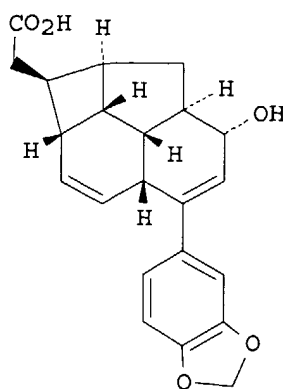
ACCESSION NUMBER: 140:196433 CA
TITLE: Endiandric acid H and its derivatives, procedures for its production and use of the same in the treatment of asthma
INVENTOR(S): Eder, Claudia; Kogler, Herbert; Haag-Richter, Sabine
PATENT ASSIGNEE(S): Aventis Pharma Deutschland Gmbh, Germany
SOURCE: Ger. Offen., 15 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
INT. PATENT CLASSIF.:
MAIN: C07D317-50
SECONDARY: A61K031-36
CLASSIFICATION: 11-1 (Plant Biochemistry)
Section cross-reference(s): 1, 26, 63
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10235624	A1	20040219	DE 2002-10235624	20020802
WO 2004014888	A1	20040219	WO 2003-EP7821	20030718
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004138313	A1	20040715	US 2003-627850	20030725
PRIORITY APPLN. INFO.:			DE 2002-10235624	20020802
			US 2003-438283P	20030106

GRAPHIC IMAGE:



I



II

ABSTRACT:

The invention concerns compds. I [R1, R2 = H, (un)branched, (un)substituted O-(C1-6-alkyl), O-(C2-6-alkenyl), O-(C2-6-alkynyl), O-(C5-10-aryl) (substituted with OH, :O, aryl, NH-(C1-6-alkyl), NH-(C2-6-alkenyl), NH2, halogen); R1R2 = O-(C1-6-alkylene)-O; R3 = H, (un)branched, (un)substituted C1-6-alkyl, C2-6-alkenyl, C2-6-alkynyl, C5-10-aryl (substituted with OH, :O, aryl, NH-(C1-6-alkyl), NH-(C2-6-alkenyl), NH2, halogen); R4 = CO2R3, CO2NHR3, CHO, CH2OR3, CH2OSi(R3)3, CH2Br, CH2CN], their stereoisomers and their physiol. acceptable salts, procedure for their production from the plant *Beilschmiedia fulva*, PLA 101037, and their use for the production of a medicament, in particular for the treatment of allergic illnesses, such as asthmatic illnesses, from inflammation associated symptoms from asthma and/or of diseases, which can be treated by restraining C-maf and NFAT. The procedure is characterized by: (1) extraction of a cell culture or the whole plant of *Beilschmiedia fulva* (PLA 101037); (2) isolation of methanoacenaphthalene II; (3) optional derivatization to I or physiol. acceptable salt formation. NFAT restraining bioassay of II gave IC50 = 1.5 μ M.

SUPPL. TERM:

Endiandric acid H deriv *Beilschmiedia fulva* isolation antiasthmatic; acenaphthalene arylmethano deriv natural product *Beilschmiedia fulva* isolation antiasthmatic; methanoacenaphthalene aryl deriv natural product *Beilschmiedia fulva* isolation antiasthmatic; C maf restraining compd Endiandric acid *Beilschmiedia fulva* isolation; NFAT restraining compd Endiandric acid *Beilschmiedia fulva* isolation

INDEX TERM:

Allergy inhibitors
Anti-inflammatory agents
Antiasthmatics
Human

(Endiandric acid H and its derivs., isolation procedures for its production and their use in the treatment of asthma)

INDEX TERM:

Transcription factors

ROLE: BSU (Biological study, unclassified); BIOL (Biological study)

(NFAT (nuclear factor of activated T-cell), inhibitors; Endiandric acid H and its derivs., isolation procedures for its production and their use in the treatment of asthma)

INDEX TERM:

Beilschmiedia fulva

(PLA 101037; Endiandric acid H and its derivs., isolation procedures for its production and their use in the treatment of asthma)

INDEX TERM:

Natural products

ROLE: NPO (Natural product occurrence); PAC (Pharmacological

activity); PRP (Properties); PUR (Purification or recovery);
THU (Therapeutic use); BIOL (Biological study); OCCU
(Occurrence); PREP (Preparation); USES (Uses)
(acenaphthalene; Endiandric acid H and its derivs.,
isolation procedures for its production and their use in the
treatment of asthma)

INDEX TERM: Transcription factors

ROLE: BSU (Biological study, unclassified); BIOL (Biological
study)
(c-maf, inhibitors; Endiandric acid H and its derivs.,
isolation procedures for its production and their use in the
treatment of asthma)

INDEX TERM: New natural products

(endiandric acid H and N, (arylmethanoacenaphthalene)
from *Beilschmiedia fulva* (PLA 101037))

INDEX TERM: Interleukin 4

ROLE: BSU (Biological study, unclassified); BIOL (Biological
study)
(human, promotor; Endiandric acid H and its derivs.,
isolation procedures for its production and their use in the
treatment of asthma)

INDEX TERM: Gene, animal

ROLE: BSU (Biological study, unclassified); BIOL (Biological
study)
(luc, IL-4 luc construct; Endiandric acid H and its
derivs., isolation procedures for its production and their
use in the treatment of asthma)

INDEX TERM: Allergy

Asthma

Inflammation

(medicinals; Endiandric acid H and its derivs., isolation
procedures for its production and their use in the treatment
of asthma)

INDEX TERM: Molecular structure, natural product

(of endiandric acid H and N, (arylmethanoacenaphthalene)
from *Beilschmiedia fulva* (PLA 101037))

INDEX TERM: 660857-93-2P, Endiandric acid H

ROLE: NPO (Natural product occurrence); PAC (Pharmacological
activity); PRP (Properties); PUR (Purification or recovery);
THU (Therapeutic use); BIOL (Biological study); OCCU
(Occurrence); PREP (Preparation); USES (Uses)
(Endiandric acid H and its derivs., isolation procedures
for its production and their use in the treatment of asthma)

INDEX TERM: 74591-03-0P, Endiandric acid A 76060-33-8P, Endiandric
acid B

ROLE: PNU (Preparation, unclassified); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(Endiandric acid H and its derivs., isolation procedures
for its production and their use in the treatment of asthma)

=>